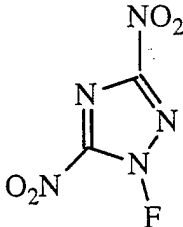


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Dr. Richard S. Miller

Technical Report No. 90

COMPUTED HEAT OF FORMATION AND IMPACT SENSITIVITY
OF A NEW DINITRO-N-FLUOROTRIAZOLE

by

Peter Politzer, J. S. Murray and M. E. Grice

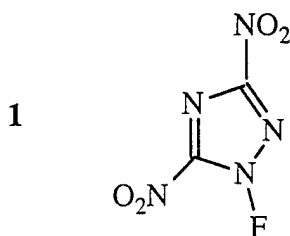
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March 7, 1996

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The dinitro-N-fluorotriazole **1** has recently been synthesized [1] and characterized crystallographically [2].



We now report our computed heat of formation and impact sensitivity for **1**.

The gas phase heat of formation was calculated using our density functional procedure [3]. It was converted to the solid phase value by means of eq. (1),

$$\Delta H_f(\text{solid}) = \Delta H_f(\text{gaseous}) - \Delta H_{\text{sub}} \quad (1)$$

in which ΔH_{sub} is the heat of sublimation. ΔH_{sub} and the impact sensitivity, h_{50} , were obtained by means of correlations that we have developed between these properties and computed quantities related to electrostatic potentials on molecular surfaces [4,5]. The latter were calculated at the *ab initio* HF/STO-5G//HF/3-21G level.

The results follow:

$$\Delta H_f(\text{gaseous}) = 77 \text{ kcal/mole} = 435 \text{ cal/gram}$$

$$\Delta H_f(\text{solid}) = 56 \text{ kcal/mole} = 316 \text{ cal/gram}$$

$$h_{50} = 126 \text{ cm}$$

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